



Aalborg Universitet

AALBORG UNIVERSITY
DENMARK

Segregation of Network Modifiers in Borosilicate Glasses

Insights from a New Transferable Potential

Wang, Mengyi; Smedskjær, Morten Matstrup; Mauro, John C.; Sant, Gaurav; Bauchy, Mathieu

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

[Link to publication from Aalborg University](#)

Citation for published version (APA):

Wang, M., Smedskjær, M. M., Mauro, J. C., Sant, G., & Bauchy, M. (2017). *Segregation of Network Modifiers in Borosilicate Glasses: Insights from a New Transferable Potential*. Abstract from 12th Pacific Rim Conference on Ceramic and Glass Technology, Waikoloa, Hawaii, United States.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal -

Take down policy

If you believe that this document breaches copyright please contact us at vbn@aub.aau.dk providing details, and we will remove access to the work immediately and investigate your claim.

Segregation of Network Modifiers in Borosilicate Glasses: Insights from a New Transferable Potential

Mengyi Wang¹, Morten M. Smedskjaer², John C. Mauro³, Gaurav Sant¹, Mathieu Bauchy¹

¹Civil and Environmental Engineering Department, University of California, Los Angeles, Los Angeles, CA, United States

²Aalborg University, Aalborg, Denmark

³Corning Incorporated, Corning, NY, USA

The existence of network modifying (alkali or alkaline-earth) atoms' segregation or clustering inside silicate glasses remains controversial. Such heterogeneity could play a crucial role in controlling macroscopic properties, including crystallization propensity, fracture, or dissolution. Here, based on molecular dynamics simulations, we report the existence of such clustering in borosilicate glasses. First, a novel inter-atomic potential was developed for modified borosilicate glasses. This new potential is found to offer an excellent transferability, as, with constant parameters, it correctly predicts the coordination number of boron atoms and the density of the glass over a wide range of Si/B ratios, from silicate to borate glasses. Predicted structure factors are also found to be in good agreement with available experimental data. Second, the simulated structures are analyzed to assess the heterogeneity of the distribution of Ca and Na atoms inside a series of borosilicate glasses. We observe a strong propensity for network modifier clustering, both for Ca and Na atoms. In turn, boron atoms are shown to enhance the homogeneity of the network. The origin of this trend is discussed.

KEYWORDS: Molecular dynamics, Borosilicate, Heterogeneity, Structure, Potential parametrization.